

CLAIMS

1. Computational data processing system, comprising an assembly of networked computers (12, ...
5 22) in each of which is stored at least one computational application, and a data processing machine (10) for storing computational data which is linked to the network and in communication with the computers (12, ... 22), at least one of the computers
10 (12) operating as master computer and at least some of the other computers (14, ... 22) operating as slave computer, characterized in that at least one of the computers (12) comprises, stored in memory, an algorithm (ClusterNtConfig) for configuring the other
15 computers of the network as slave computers and an executable master application for managing the tasks of each slave computer as a function of their availability for the assignment, to each of them, of computational tasks and of corresponding computational data which are
20 stored in the storage machine (10).
2. System according to Claim 1, characterized in that the said configuring algorithm and the said master application are loaded into each computer (12, ... 22) of the network, the execution of the said configuring
25 algorithm by one of the computers constituting a means of configuring the latter as master computer.
3. System according to Claim 2, characterized in that each computer furthermore comprises an executable slave application under the control of the master
30 computer (12) when this computer is configured as slave, for the local management of the computational application, the said slave application comprising software means for talking to the storage machine (10).
4. System according to Claim 3, characterized in
35 that the said software means for talking to the storage machine comprise means for exchanging data according to a file transfer protocol.
5. System according to Claim 1, characterized in that each master computer (12) comprises, stored in

memory, an electronic signature and means for comparing the said signature and an electronic signature of a slave computer with which it communicates so as to authorize the running of the computational application

5 by the latter computer.

6. System according to Claim 1, characterized in that the configuring algorithm comprises software means for formulating a man/machine interface (24) suitable for display on a screen of each computer for the

10 configuring of the said computers.

7. Process of computation by means of a data processing system according to any one of Claims 1 to 6, characterized in that it comprises the steps of:

defining at least one group of computers by

15 configuring for each group a computer (12, ... 22) as master computer and other computers as slave computers;

assigning, to each of the slave computers, one or more computational applications and corresponding computational data;

20 comparing an electronic signature sent by each slave computer to the master computer with a corresponding signature stored in the latter; and in the case of correspondence between the said signatures:

running, for each slave computer, the

25 computational application or applications as a function of their availability, using the corresponding computational data; and

retrieving the data resulting from the execution of the applications carried out in parallel,

30 in each slave computer.

8. Use of a computational process according to Claim 7 for the computation of molecular models on the basis of molecular data stored in a data server (10).